

Identifying the closeness of eigenstates in quantum many-body systems

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We propose a new quantity called modulus fidelity to measure the closeness of two quantum pure states. Especially, we use it to investigate the closeness of eigenstates of quantum many-body systems. When the system is integrable, the modulus fidelity of neighbor eigenstates displays a large fluctuation. But the modulus fidelity is close to a constant when system becomes non-integrable with fluctuation reduced drastically. Average modulus fidelity of neighbor eigenstates increases with the increase of parameters that destroy the integrability, which also indicates the integrable-chaos transition. In non-integrable case, it is found two eigenstates are closer to each other if their level spacing is small. We also show that the closeness of eigenstates in non-integrable domain is the underlying mechanism of *eigenstate thermalization hypothesis* (ETH) which explains the thermalization in nonintegrable system we studied.

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INTRODUCTION

Statistical mechanic has succeeded in describing quantum many-body system. But how to understand thermodynamics from quantum mechanics remains an unsolved problem in physics. We speak of ‘thermalization’ for an isolated quantum many-body system when it reaches a steady state that can be described by an equilibrium thermodynamic ensemble and the expectation values of observables are time-independent at this steady state. Recently, the ground breaking experimental progress in preparing and manipulating ultracold atomic quantum gases [1] have made it possible to obtain a system weakly coupled with the environment. These approximately isolated systems are ideal test beds for the investigation of relaxation and thermalization. It is found that the relaxation to equilibrium surely takes place [2] in certain setups but fails to be approached in others [3]. These experimental results stimulate intense theoretical effort to find the condition under which thermalization of quantum system can be approached.

Integrability is believed to be the intrinsic mechanism of the failure of thermalization in one-dimensional boson system [4]. It is also found that the breaking of integrability is related to the onset of thermalization. On the other hand, quantum chaos will emerge in the breaking of integrability when the perturbation is strong enough. Then, the link between quantum chaos and thermalization seems to be established. As well known, quantum chaos is used to address some properties of quantum system whose classic counterparts are chaotic. It is found that the properties of spectra, eigenstate and dynamics of quantum system can indicate the emergence of quantum chaos. Most of these studies focus on the statistical properties [5–9]. An important description of energy level is level spacing distribution $P(s)$, which is the probability distribution of the distances between consecutive levels $s_i = E_{i+1} - E_i$, where s_i is normalized to unit as $\langle s \rangle = 1$. At integrability, $P(s)$ is a typically Poisson distribution $P(s) = e^{-s}$ while at chaos the distribution takes the Wigner-Dyson form $P(s) = (\pi/2)se^{-\pi s^2/4}$ [5, 10]. Consider the eigenstate expanded in certain basis, the distribution of coefficient was shown to be localized or extended, which is related to the integrable-chaos transition to some degree. In latter case, eigenstates are chaotic wavefunction [11, 12] and they are similar because of similar structure [7, 8], which is a kind of statistical similarity. However, despite intense studies, what is the nature of the integrable-chaos transition is still unclear.

For an isolated quantum many-body system with Hamiltonian H , the eigenstate thermalization hypothesis (ETH) [13] states that thermalization occurs in individual eigenstates. That is to say, let $|\Psi_i\rangle$ denote an eigenstate of the system with eigenvalue E_i and let A denote a few-body observable, then the equation

$$\langle \Psi_i | A | \Psi_i \rangle = \langle A \rangle_{micro}(E_i) \quad (1)$$

is satisfied, where the subscript *micro* denotes the microcanonical thermal average over the energy interval $[E_i - \Delta E/2, E_i + \Delta E/2]$, where ΔE is the energy interval. ETH has been verified numerically in a wide variety of quantum many-body systems which are far from integrability [7, 8, 14, 15]. Recently, it was shown [16] that ETH is essentially equivalent to the basic assumption of von Neumann’s quantum ergodic theorem (QET) [17]

ETH which shows the closeness of expectation value of observable on energy eigenstate motivates us to study a definite closeness of energy eigenstates close in energy, other than statistical similarity. The intrinsic and widely used tool to investigate the closeness of two states, including pure state and mixed state, in quantum information

theory is fidelity F [18]. As previously discussed, experiment setup can prepare isolated quantum many-body system which is described by a single wave function according to quantum mechanics. Therefore, in the following, we just consider pure state. Assuming two pure states denoted by $|\Phi\rangle$ and $|\Psi\rangle$, the fidelity of these two states is defined as $F(|\Phi\rangle, |\Psi\rangle) = |\langle\Phi|\Psi\rangle|$. If these two states are identical, $|\Phi\rangle = |\Psi\rangle$ or differ by a global phase as $|\Phi\rangle = e^{i\theta}|\Psi\rangle$, then $F = 1$. If they are orthogonal, $F = 0$. As all eigenstates of one quantum many-body system are orthogonal, the fidelity of each pair of eigenstates are all zero no matter what this system is, integrable or nonintegrable, then we cannot use fidelity to define and study the closeness of eigenstates of quantum many-body system in this sense. To study the substantial properties of quantum many-body system, for example, the transition from integrable to chaos, we should build a new understanding of closeness of quantum states.

This article is organized as follows. In Sec. II, we introduce a new measurement called modulus fidelity. In Sec. III, we use modulus fidelity to investigate the transition from integrable to chaos in one-dimensional quantum many-body system. In Sec. IV, based on numerical results, we provide an understanding of the origin of ETH. Finally, we summarize our results in V.

THE DEFINITION OF MODULUS FIDELITY

In this paper, we propose a new measurement to define and identify the closeness of two quantum states which are the eigenstates of an isolated quantum many-body system with Hamiltonian H . We still denote them by $|\Phi\rangle$ and $|\Psi\rangle$. Let $|n_i\rangle$ denotes a complete orthogonal set in Hilbert space of this quantum system with dimension L . This orthogonal basis is arbitrary in Hilbert space and can be assumed as the eigenstates of an observable A with eigenvalue a_i . Then $|\Phi\rangle$ and $|\Psi\rangle$ can be expanded as $|\Phi\rangle = \sum_{i=1}^L c_i |n_i\rangle$, and $|\Psi\rangle = \sum_{j=1}^L d_j |n_j\rangle$, where $c_i(d_j)$ is the expansion coefficient. The fidelity of these two states is $F = \sum_{i=1}^L c_i^* d_i$. If we measure A on the state $|\Psi\rangle$, then the probability of obtaining eigenvalue a_i is $|c_i|^2$. After repeating measurement, one can get all eigenvalues with a sequence of probability $\{|c_1|^2, |c_2|^2, \dots, |c_L|^2\}$. Doing same measurement on state $|\Phi\rangle$, we can get another sequence $\{|d_1|^2, |d_2|^2, \dots, |d_L|^2\}$. To identify the closeness of two states by comparing these two sequences, we use a measure in the form of fidelity as

$$F_m = \sum_{i=1}^L |c_i| |d_i| \quad (2)$$

where the modulus operation is to make the value of F_m in $[1, 0]$ as well as fidelity and we call F_m modulus fidelity. Such measure is similar with the one used in ref. [9?] where the product of square of modulus of expansion coefficient were summed.

To better understand this new measure, we construct a new kind of vectors in the same Hilbert space $|n_i\rangle$ by setting its coefficients as the modulus of the coefficients of a vector like $|\Phi\rangle$. Then the new vectors built on $|\Phi\rangle$ and $|\Psi\rangle$, denoting by $|\tilde{\Phi}\rangle$ and $|\tilde{\Psi}\rangle$, are defined as

$$\begin{aligned} |\tilde{\Phi}\rangle &= \sum_i^L |c_i| |n_i\rangle, \\ |\tilde{\Psi}\rangle &= \sum_j^L |d_j| |n_j\rangle. \end{aligned} \quad (3)$$

then F_m of two pure states $|\Phi\rangle$ and $|\Psi\rangle$ is the fidelity of $|\tilde{\Phi}\rangle$ and $|\tilde{\Psi}\rangle$ as

$$F_m(|\Phi\rangle, |\Psi\rangle) = |\langle\tilde{\Phi}|\tilde{\Psi}\rangle| = \langle\tilde{\Phi}|\tilde{\Psi}\rangle. \quad (4)$$

In last equality, the modulus operation vanishes due to the definition of new state (3). Note that F_m has the same definition as fidelity, but it is defined in new constrained space, describing the overlap of two quantum pure states in terms of modulus of coefficient. Modulus fidelity has some different properties from fidelity, for example, it is dependent on the choice of basis, while fidelity is independent. Such replacing coefficients by their modulus was also proposed recently in ref. [19] to study its effect on entanglement entropy.

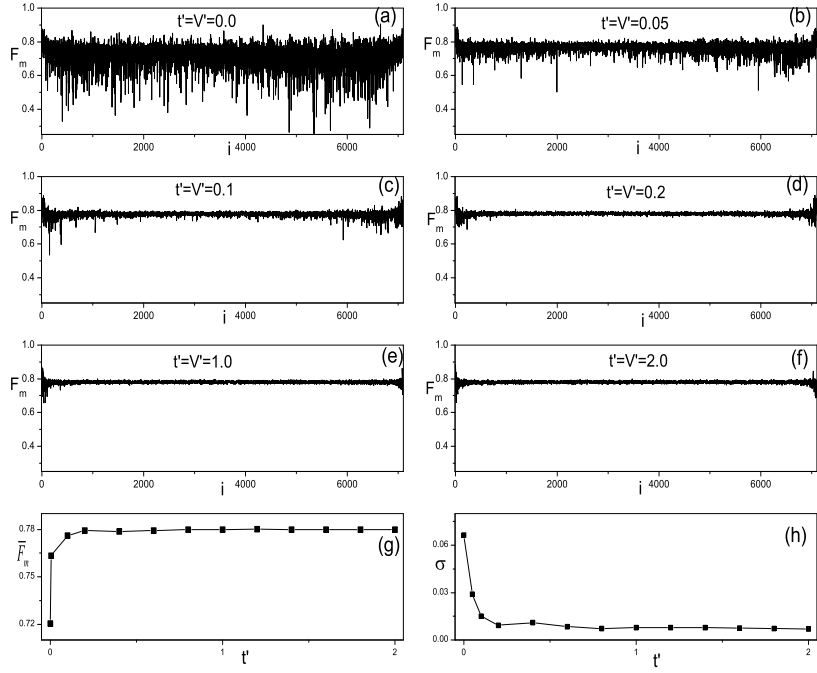


FIG. 1: The modulus fidelity $F_m(i, i-1)$ of i th eigenstates and $(i-1)$ th eigenstate in 1-D hard-core model. The data are obtained in the condition that 6 bosons on 25 lattice and the next-nearest-neighbor parameters are changed from (a) integrable case to nonintegrable case (b)-(f). Average modulus fidelity (g) and the standard deviation of modulus fidelity (h) of neighbor eigenstates in present model as a function of the next-nearest-neighbor hopping parameters $t' = V'$.

NUMERICAL RESULTS

In the following, we use modulus fidelity F_m to study the closeness of eigenstates of a quantum many-body system in both integrable and nonintegrable domain. We consider one-dimensional hard-core boson model(HCB) with dimensionless Hamiltonian

$$H = \sum_{i=1}^N \{-t(\hat{b}_i^\dagger \hat{b}_{i+1} + H.c.) - t'(\hat{b}_i^\dagger \hat{b}_{i+2} + H.c.) + V\hat{n}_i \hat{n}_{i+1} + V'\hat{n}_i \hat{n}_{i+2}\},$$

where t and t' are the nearest-neighbor hopping and the next-nearest-neighbor hopping, V and V' are the nearest-neighbor and the next-nearest-neighbor interaction respectively. Throughout this paper, t and V are set to be unit, $t = V = 1$, and t' and V' are set to be equal, $t' = V'$. $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is density operator. As well known, this model is integrable when $t' = V' = 0.0$ but nonintegrable when $t' = V' \neq 0.0$. It has been verified that the thermalization can be achieved in this system and the underlying mechanism is ETH when system is far from integrable [7, 14, 15].

We use full exact diagonalization method to calculate all eigenstates and eigenvalues of present system. We study the lattice up to 25 sites and 6 hard-core bosons. Under period boundary condition, the system preserves translational symmetry, by which the Hilbert space of Hamiltonian can be decomposed into different independent subspace with different total momentum k . We can diagonalize each subspace. As discussed above, modulus fidelity is dependent on the choice of basis. That is to say, for two eigenstates we consider, the values of modulus fidelity is different in different basis. However, as the number of eigenstates of many-body quantum system is large, we can focus on the statistical properties of modulus fidelity of eigenstates. We investigate the modulus fidelity in two different basis, site basis(Fock state) and k basis(Bloch state). These two bases were used to study the localization of a single eigenstate of quantum many-body system in integrable-chaos transition.

In our simulation, we found that the statistical properties of modulus fidelity are the same in these two kinds of bases. Throughout this paper, we just illustrate the results of modulus fidelity obtained in site basis. The eigenstates in illustration are obtained in subspace with momentum $k = 1$ rather than $k = 0$ to avoid a parity symmetry. Then they are transformed into to space of site basis.

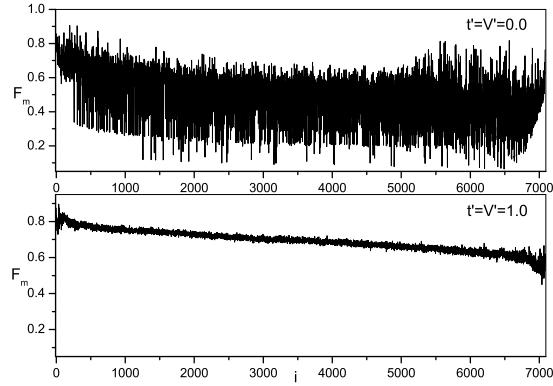


FIG. 2: The modulus fidelity of excited states with the ground state. (a) $t' = V' = 0.0$ and (b) $t' = V' = 1.0$.

We first calculate F_m of neighbor eigenstates in subspace at different values of the next-nearest neighbor hopping and interaction which determines the breaking of integrability in the system. The numerical results are plotted in Fig.1. Note that when $t' = V' = 0$, i.e., the system is integrable, as shown in Fig.1(a), each modulus fidelity F_m of the pair of neighbor eigenstates is non-zero, and most of them are larger than 0.5, which means, on the whole, that in integrable case eigenstates are close to their neighbor ones in term of modulus fidelity. The most significant feature is that they have large fluctuation. F_m distribute along the eigenvalues like random number in an interval with large fluctuation. When t' and V' are non-zero, the system becomes nonintegrable. As is well known, the level spacing distribution changes from Poisson to Wigner-Dyson form, indicating a transition from integrable to chaos. In Fig.1 (b-f), we found that the values of modulus fidelity between most neighbor eigenstates are also larger than 0.5 and vary round a constant as well as the case of integrability. However, there is a dramatic change appearing that the fluctuation of modulus fidelity is reduced with the increase of t' and V' . When t' and V' is large enough, for example, $t' = V' = 2.0$ in Fig.1(f), as a function of index of eigenvalues, F_m is no longer like random number, but tends to be a smooth constant. That is to say, when the system comes into chaos, most of eigenstates of system becomes close to their neighbor one in term of modulus fidelity and the values of the modulus fidelity also become close so that eigenstates are close to each other.

We also calculate the average modulus fidelity of all modulus fidelity between pair neighbor eigenstates, $\bar{F}_m = \frac{1}{L-1} \sum_{i=1}^{L-1} F_m(i)$, where L is the size of subspace, and the standard deviation. The results are also plotted in Fig 1. We can see obvious changes in both measures. When t' and V' increase from zero, i.e., integrability point, average modulus fidelity increases quickly. In Fig.1(a-f), we have found all eigenstates become close to each other when system is far from integrability. Here, we find that the degree of closeness of eigenstates will also increase in this process. After t' and V' reach a certain value, average modulus fidelity will not increase so quickly and almost tends to be saturated. For the parameters of model we investigated here, this value is about 0.25. This scenario can also be seen in the results of standard deviation of modulus fidelity. It decreases very quickly when t' and V' increase from zero, which indicates the reduction of fluctuation seen in Fig.1(a-f). The reduction of fluctuation was also found in ref. [9] by using a similar measure as discussed above. But except for this result, the closeness are measured differently. In ref. [9], maximal value of overlap(closeness) decrease when system becomes nonintegrable, which is contrary to our result. When t' and V' are large enough and system comes into chaos, the fluctuation is inhibited to be small and decreases slowly as confirmed in Fig.1(h). The values of t' and V' at which transition occurs are the same as that of the average modulus fidelity. The existence of such critical values has been found [4, 7, 15] and they will decrease with the increase of size of system. So it is believed that in the thermodynamic limit an infinitesimal integrability breaking would lead to chaos.

As shown previously, when system is in integrable and nonintegrable cases, the statistical properties of modulus fidelity of neighbor eigenstates behave differently. Next, we provide further evidence for this statement. We choose ground state as a reference state and calculate modulus fidelity of excited eigenstates with respect to it. We plot some results of modulus fidelity as a function of the index of eigenstate in Fig.2. Both in integrable case and nonintegrable case, the overall trend of modulus fidelity of excited state with respect to ground state decreases when the excited state is far from ground state in energy. However, the local details in two case are different. We also notice a reduction of fluctuation appearing in such modulus fidelity as well as modulus fidelity of neighbor eigenstates shown in Fig.1. In

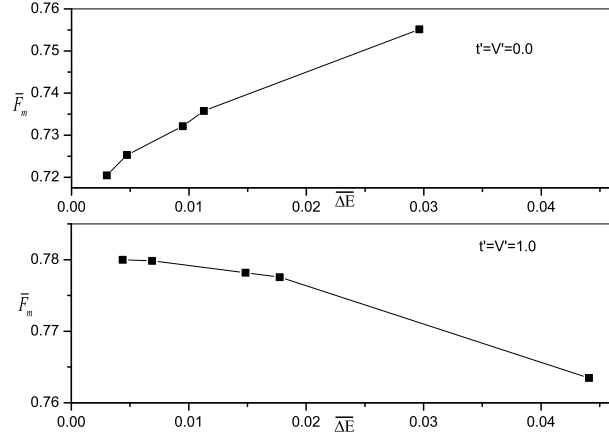


FIG. 3: Average modulus fidelity versus average level spacing (energy density) for 1-D hard-core boson system with (a) $t' = V' = 0.0$ and (b) $t' = V' = 1.0$. Average level spacings $\overline{\Delta E}$ are obtained by $(E_{max} - E_{min})/N$ where E_{max} and E_{min} are the two ends of energy spectrum.

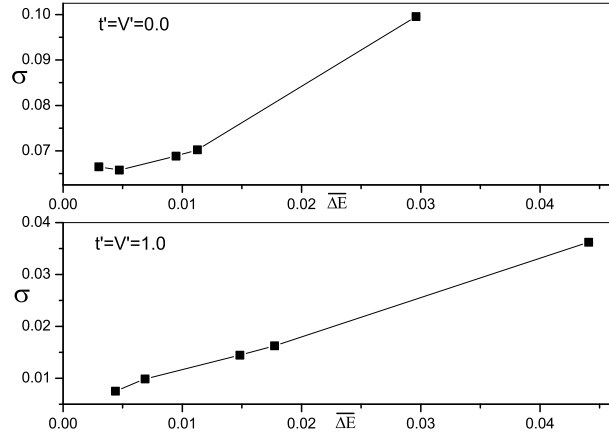


FIG. 4: Standard deviation versus average level spacing (energy density) for 1-D hard-core boson system with (a) $t' = V' = 0.0$ and (b) $t' = V' = 1.0$. Average level spacings $\overline{\Delta E}$ are obtained by $(E_{max} - E_{min})/N$ where E_{max} and E_{min} are the two ends of energy spectrum.

integrable case, there is also a large fluctuation presenting along the function of modulus fidelity. That is to say, there is no clear relation between closeness and level spacing. When system is nonintegrable, the fluctuation is reduced sharply and modulus fidelity of excited state with respect to ground state becomes a smooth function of index of eigenstate. That is to say, the closeness of two states and level spacing are in inverse proportion, i.e., the small level spacing is, the more close two states become. The eigenvalues of one Hamiltonian have a nature order, varying from minimum to maximum. Due the results show in Fig.1 and Fig.2, we find that at chaos such order of eigenvalues has its counterpart in eigenstates, which is described by the modulus fidelity. However, this relationship is destroyed in integrable case, by which we can also distinguish the integrable and chaos domain in a quantum many-body system.

Next, we investigate the relation between the closeness of eigenstates and level spacing by changing the system size. As well known, in the thermodynamic limit, the level spacing of quantum many-body is expected to be zero. For a finite system, level spacings between each pair of neighbor eigenstates are not the same and obey a distribution. To compare the closeness at different system size, we calculate average modulus fidelity of neighbor eigenstates. Accordingly, level spacings are also averaged. In Fig.3, we plot numerical results of system in both integrable and nonintegrable cases. When system is integrable, average modulus fidelity decrease with the decrease of energy level, which means the close of energy level lead to the separation of corresponding eigenstates. But in nonintegrable case, average modulus fidelity increases with the decrease of level spacing, showing that when eigenstates become close in

energy, they will be close in term of modulus fidelity as well as in Fig.2. The standard derivation of modulus fidelity of neighbor eigenstates in different system size are plotted in Fig.4. When system is nonintegrable, standard derivation decreases with the decrease of level spacing, i.e., the increase of system size. That is to say, when system size becomes large, the closeness of neighbor eigenstates tends to be the smooth function of energy. When system is integrable, standard derivation also decreases as the the system size increase for most data, except for the one when system size takes maximal value in our study. In the future work, a large scale simulation should be done to find whether it is a error or a intrinsic character of integrable system.

THE UNDERLYING MECHANISM OF EIGENSTATE THERMALIZATION HYPOTHESIS

We have identify the integrable-chaos transition in quantum many body system which is related to the emergence of thermalization. As ETH states, when system is at chaos, the expectation value of the observable A on energy eigenstate $|\Phi_i\rangle$, $\langle\Phi_i|A|\Phi_i\rangle$, is a smooth function of eigenvalues E_i . One can expand eigenstate $|\Phi_i\rangle$ by another orthogonal complete basis which could be constructed by the eigenstates of observable A . If A commutes with Hamiltonian, its eigenstates are the same as that of Hamiltonian, so $|\Phi_i\rangle$ is expanded on itself. In this case, F_m is zero for any pairs of eigenstates, which is trivial for studying the closeness of eigenstate as well as fidelity F . We focus on the case that observable A doesn't commute with Hamiltonian. For the quantum system we considered, assume an eigenstate of observable A is $|\alpha_l\rangle$ with eigenvalues a_l , i.e., $A|\alpha_l\rangle = a_l|\alpha_l\rangle$. Let $|\Phi_i\rangle$ and $|\Phi_{i-1}\rangle$ denote two eigenstates of Hamiltonian close in energy, then they can be expanded by the eigenstates of observable A as $|\Phi_i\rangle = \sum_l \beta_{i,l}|\alpha_l\rangle$, $|\Phi_{i-1}\rangle = \sum_l \beta_{i-1,l}|\alpha_l\rangle$ where $\beta_{n,l}$ is coefficient. Then the expectation value of A on these two eigenstates are

$$\begin{aligned}\langle\Phi_i|A|\Phi_i\rangle &= \sum_l |\beta_{i,l}|^2 a_l. \\ \langle\Phi_{i-1}|A|\Phi_{i-1}\rangle &= \sum_l |\beta_{i-1,l}|^2 a_l.\end{aligned}\tag{5}$$

where $|\beta_{i,l}|^2 = \beta_{i,l}^* \beta_{i,l}$ is the eigenstate occupation numbers which is the probability of obtaining the eigenvalue a_l in a measurement of A on energy eigenstate $|\Phi_i\rangle$. In nonintegrable case, due to Eq.(1) of ETH, $A(E)$ equals to microcanonical average, which means

$$\langle\Phi_i|A|\Phi_i\rangle \approx \langle\Phi_{i-1}|A|\Phi_{i-1}\rangle.\tag{6}$$

Due to Eq. (5), one can find the valid of Eq. (6) is contributed by two properties, the eigenvalues of A and eigenstate occupation number. As the former is fixed for a quantum system, then there should be two possible scenario for eigenstate occupation number ($|\beta_{n,l}|^2$) that they fluctuate between eigenstate close in energy or not. Now, our result that in nonintegrable system we studied the modulus fidelity has larger value and keeps almost constant suggests the later that for two eigenstates of Hamiltonian close in energy, the eigenstate occupation number of them are also close as

$$|\beta_{i,l}|^2 \approx |\beta_{i-1,l}|^2.\tag{7}$$

Then the Eq. (6) will be satisfied. In this case, the modulus fidelity between each pair of neighbor eigenstate will tend to be unit and equal to each other, showing a smooth function versus eigenvalues. On the contrary, if the expansion coefficient $|\beta_{n,l}|^2$ is fluctuating between eigenstates close in energy, i.e., Eq. (7) is violated, the modulus fidelity between pair neighbor eigenstates will have a fluctuation as shown in Fig.1 to Fig.3. In ref.[16], the basis of ETH and QET is assumed that the overlap between an energy eigenstate and an eigenstate of an observable A is exponential small and close to $\frac{1}{D}$, where D is the dimension of Hilbert space of system. It can be found here that this assumption is an extreme point in our result that will also make modulus fidelity to be unit.

CONCLUSION

In conclusion, we found that the closeness of eigenstates of Hamiltonian of quantum many-body system can be studies as an indicator for the transition from integrability to chaos. For this purpose, we proposed a new measure, modulus fidelity, which is defined by replacing the expansion coefficients of one quantum state in a basis by

their modulus. The full exact diagonalization of one-dimensional hard-core boson model showed that in integrable and nonintegrable case, the modulus fidelity of neighbor eigenstates have different properties, which indicates the integrable-chaos transition. The reduction of fluctuation of modulus fidelity and the increase of their average value in this transition show the eigenstates of quantum many body system tend to be close to each other, which show a deeper uniformization of eigenstates than statistical similarity. We also studied the finite effect on such transition. Furthermore, our analysis show the closeness of eigenstate guarantees the valid of ETH in nonintegrable system we studied and suggest a general understanding of the underlying mechanism of ETH and QET.

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